

Quantum Decoherence at Finite Temperatures

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We study measures of decoherence and thermalization of a quantum system S in the presence of a quantum environment (bath) E . The whole system is prepared in a canonical thermal state at a finite temperature. Applying perturbation theory with respect to the system-environment coupling strength, we find that under common Hamiltonian symmetries, up to first order in the coupling strength it is sufficient to consider the uncoupled system to predict decoherence and thermalization measures of S . This decoupling allows closed form expressions for perturbative expansions for the measures of decoherence and thermalization in terms of the free energies of S and of E . Numerical results for both coupled and decoupled systems with up to 40 quantum spins validate these findings.

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Decoherence and thermalization are two basic concepts in quantum statistical physics [1]. Decoherence renders a quantum system classical due to the loss of phase coherence of the components of a system in a quantum superposition via interaction with an environment (or bath). Thermalization drives the system to a stationary state, the (micro) canonical ensemble via energy exchange with a thermal bath. As the evolution of a quantum system is governed by the time-dependent Schrödinger equation, it is natural to raise the question how classicality could emerge from a pure quantum state. This question is becoming more important technologically, for example in designing quantum computers [2] where decoherence effects are a major impediment in engineering implementations.

Various theoretical and numerical studies have been performed, trying to answer this fundamental question, *e.g.*, the microcanonical thermalization of an isolated quantum system [3–6], canonical thermalization of a system coupled to a (much) larger environment [3, 7–17], and of two identical quantum systems at different temperatures [18, 19]. In our earlier work [20], we found that at infinite temperature the degree of decoherence of a system S scales with the dimension of the environment E if the state of the whole system $S + E$ is randomly chosen from the Hilbert space of the whole system. We showed that in the thermodynamic limit, the system S decoheres thoroughly.

In this Letter, we investigate for the first time quantitatively how classicality emerges from a pure quantum state when $S + E$ is of a finite size and at a finite temperature. We assume that the whole system $S + E$ is in a canonical thermal

state, a pure state at finite inverse temperature β [21–23], and investigate measures of the decoherence and the thermalization of S . This canonical thermal state could be the result of a thermalization process of the whole system $S + E$ coupled to a large heat bath, which we do not consider any further. The state of the system S is described by the reduced density matrix. The degree of decoherence of the system S is measured in terms of σ , defined below in terms of measures of the off-diagonal components of the reduced density matrix. If $\sigma = 0$, then the system S is in a state of full decoherence. The difference between the diagonal elements of the reduced density matrix and the canonical or Gibbs distribution is expressed by δ . Hence, for a system being in its canonical distribution it is expected that both σ and δ are zero. We show that under symmetry transformations that leave the Hamiltonians of S and E invariant but reverse the sign of the interaction Hamiltonian, conditions which are usually satisfied for example in quantum spin systems, the first-order term of the perturbation expansion of σ^2 in terms of the interaction between S and E is exactly zero. Therefore it is sufficient to study the uncoupled system. We demonstrate that the leading term in the expressions for σ^2 and δ^2 is a product of factors of the free energy of E and the free energy of S . Hence, these expressions for σ^2 and δ^2 allow one to study the influence of the environment on the decoherence and thermalization of S . We study the validity region of these results obtained from perturbation theory by performing large-scale simulations for spin-1/2 systems with initial states from a canonical thermal state.

The Hamiltonian of the whole system $S + E$ can be ex-

pressed as

$$H = H_S + H_E + \lambda H_{SE}, \quad (1)$$

where H_S and H_E are the system and environment Hamiltonian, respectively, and λH_{SE} describes the interaction between the system S and environment E . Here λ denotes the global system-environment coupling strength.

The state of the system S is described by the reduced density matrix $\hat{\rho} \equiv \text{Tr}_E \rho$, where $\rho = |\Psi\rangle\langle\Psi|$ is the density matrix of the whole system $S + E$ and Tr_E denotes the trace over the degrees of freedom of the environment E . The state of the whole system $S + E$ can be written as $|\Psi\rangle = \sum_{i=1}^{D_S} \sum_{p=1}^{D_E} c(i, p) |i, p\rangle$, where the set of states $\{|i, p\rangle\}$ denotes a complete set of orthonormal states in some chosen basis, and D_S and D_E are the dimensions of the Hilbert spaces of the system S and environment E , respectively. We assume that D_S and D_E are both finite and $D = D_S D_E$ is the dimension of the Hilbert space of the whole system $S + E$. In terms of the expansion coefficients $c(i, p)$, the matrix element (i, j) of the reduced density matrix reads $\hat{\rho}_{ij} = \sum_{p=1}^{D_E} c^*(i, p) c(j, p)$.

We characterize the degree of decoherence of the system S by [11]

$$\sigma = \sqrt{\sum_{i=1}^{D_S-1} \sum_{j=i+1}^{D_S} |\tilde{\rho}_{ij}|^2}, \quad (2)$$

where $\tilde{\rho}_{ij}$ is the matrix element (i, j) of the reduced density matrix $\hat{\rho}$ in the representation that diagonalizes H_S . Clearly, σ is a global measure for the size of the off-diagonal terms of $\tilde{\rho}$. If $\sigma = 0$ the system is in a state of full decoherence (relative to the representation that diagonalizes H_S). We define a quantity measuring the difference between the diagonal elements of $\tilde{\rho}$ and the canonical distribution as [11]

$$\delta = \sqrt{\sum_{i=1}^{D_S} \left(\tilde{\rho}_{ii} - e^{-bE_i^S} / \sum_{i=1}^{D_S} e^{-bE_i^S} \right)^2}, \quad (3)$$

where $\{E_i^S\}$ denote the eigenvalues of H_S and b is a fitting inverse temperature. The quantities σ and δ are respectively general measures for the decoherence and thermalization of S .

A canonical thermal state is a pure state at a finite inverse temperature β defined by (the imaginary-time projection) [21–23]

$$|\Psi(\beta)\rangle = e^{-\beta H/2} |\Psi(0)\rangle / \langle \Psi(0) | e^{-\beta H} | \Psi(0) \rangle^{1/2}, \quad (4)$$

where $|\Psi(0)\rangle = \sum_{i=1}^D d_i |i\rangle$ and $\{d_i\}$ are complex Gaussian random numbers. The justification of this definition can be seen from the fact that for any quantum observable A of the whole system [21, 23], one has $\langle \Psi(\beta) | A | \Psi(\beta) \rangle \approx \text{Tr} A e^{-\beta H} / \text{Tr} e^{-\beta H}$. The error in the approximation is of the order of the inverse square root of the Hilbert space size of the whole system [21] and therefore the approximation improves for increasing D . One may consider the state $|\Psi(\beta)\rangle$

as a “typical” canonical thermal state [23] in the sense that if one measures observables, their expectation values agree with those obtained from the canonical distribution at the inverse temperature β . In the following we present analytical results for σ and δ when the whole system $S + E$ is in such a state $|\Psi(\beta)\rangle$.

The system S is coupled to an environment E with global coupling strength λ , and therefore we resort to perturbation theory with respect to λ . Up to first order in the global system-environment coupling strength λ , we have [24]

$$e^{-\beta H} \approx \left(1 - \left\{ \int_0^1 d\xi e^{-\beta \xi H_0} H_{SE} e^{\beta \xi H_0} \right\} \beta \lambda \right) e^{-\beta H_0}, \quad (5)$$

where $H_0 = H_S + H_E$ denotes the Hamiltonian of the uncoupled system and bath. If we now consider a unitary transformation that leaves H_S and H_E invariant but reverses the sign of H_{SE} , then $\langle \Psi(0) | e^{-\beta H} | \Psi(0) \rangle \approx \text{Tr} e^{-\beta H_0} / D = Z_0 / D$, where Z_0 denotes the partition function of the uncoupled system. The expression Eq. (4) for the canonical thermal state becomes

$$|\Psi(\beta)\rangle \approx \sqrt{\frac{D}{Z_0}} e^{-\beta H/2} |\Psi(0)\rangle. \quad (6)$$

Using Eq. (5) and Eq. (6), we find that the first-order term of the perturbation expansion in λ of the expectation value of σ^2 is given by

$$\begin{aligned} \langle \langle \sigma^2 \rangle \rangle_1 &= -\beta \lambda \left(\frac{D}{Z_0} \right)^2 \frac{D}{D+1} \\ &\times \left[Z_S \text{Tr} e^{-\beta H_S} e^{-2\beta H_E} H_{SE} - \text{Tr} e^{-2\beta H_0} H_{SE} \right], \end{aligned} \quad (7)$$

where $Z_S = \text{Tr} e^{-\beta H_S}$. Here and in the following $\langle \langle \cdot \rangle \rangle$ denotes the expectation value with respect to the probability distribution of the random numbers $\{d_i\}$. Applying the same unitary transformation as discussed before results in $\langle \langle \sigma^2 \rangle \rangle_1 = 0$. Hence, to study the decoherence of a system S coupled to an environment E up to first order in λ it is *sufficient to study the uncoupled system* ($\lambda = 0$). Furthermore, one state of the type Eq. (4) is enough to get the correct expectation value provided the dimension of the Hilbert space is large [21].

Therefore, we now focus on the uncoupled system. There exist simple relations for the eigenvalues E_j (eigenstates $|E_j\rangle$) of the Hamiltonian H in terms of the eigenvalues E_i^S , E_p^E (eigenstates $|E_i^S\rangle$, $|E_p^E\rangle$) of the system Hamiltonian H_S and environment Hamiltonian H_E , respectively, i.e., $E_j = E_i^S + E_p^E$ and $|E_j\rangle = |E_i^S\rangle |E_p^E\rangle$. We first perform a Taylor series expansion of σ^2 up to second order in $|d|^2$ about the point $1/D$ and then calculate the expectation value of σ^2 . A lengthy calculation gives

$$\begin{aligned} \langle \langle \sigma^2 \rangle \rangle &= \frac{1}{2} e^{-2\beta(F_E(2\beta) - F_E(\beta))} \left(1 - e^{-2\beta(F_S(2\beta) - F_S(\beta))} \right) \\ &- \frac{2D}{D+1} e^{-3\beta(F_E(3\beta) - F_E(\beta))} \\ &\times \left(e^{-2\beta(F_S(2\beta) - F_S(\beta))} - e^{-3\beta(F_S(3\beta) - F_S(\beta))} \right) \end{aligned}$$

$$+ \frac{3D}{2(D+1)} e^{-4\beta(F_E(2\beta)-F_E(\beta))} e^{-2\beta(F_S(2\beta)-F_S(\beta))} \times \left(1 - e^{-2\beta(F_S(2\beta)-F_S(\beta))}\right), \quad (8)$$

where $F_S(n\beta)$ and $F_E(n\beta)$ represent the free energy of the system S and the environment E at the inverse temperature $n\beta$, respectively. Obviously, in most of the cases the first term dominates.

Two special cases are of interest. First, if $\beta = 0$, we recover the previous result $E(\sigma^2) = (D_S - 1)/2(D+1)$ [20]. In the vicinity of $\beta = 0$, the first-order term of the Taylor expansion of Eq. (8) vanishes. Hence in the high temperature limit, $\langle\langle\sigma^2\rangle\rangle = (D_S - 1)/2(D+1) + \mathcal{O}(\beta^2)$.

If the temperature approaches zero, Eq. (8) becomes

$$\lim_{\beta \rightarrow \infty} \langle\langle\sigma^2\rangle\rangle = \frac{g_S - 1}{2g_S g_E} \left(1 - \frac{D_S D_E}{(D_S D_E + 1)g_S g_E}\right), \quad (9)$$

where g_S and g_E refer to the degeneracy of the ground state of the system S and environment E , respectively. This expression yields zero if the ground state of the system is non-degenerate. For a system with a highly degenerate ground state ($g_S \gg 1$) the expression goes to $1/2g_E$. For a system with known $g_S > 1$ and a large environment $D_E \gg 1$, at small λ and at low temperatures, if one measures $\langle\langle\sigma^2\rangle\rangle$, one can determine the degeneracy g_E of the ground state of the environment. This is a new, strong prediction. The ground state degeneracy g_E of the environment can be estimated by only measuring quantities in S . Furthermore, Eq. (9) should be a guide to engineering quantum systems that have limited decoherence at low temperatures, namely systems with large g_S (one characteristic of topological quantum computation [25]) but non-degenerate g_E so $\langle\langle\sigma^2\rangle\rangle \approx 1/2$.

Similarly, we can make the Taylor expansion for δ^2 up to second order with respect to both $|d|^2$ and b about the points $1/D$ and β . The expectation value of δ^2 is given by

$$\begin{aligned} \langle\langle\delta^2\rangle\rangle = & \frac{D}{D+1} e^{-2\beta(F_E(2\beta)-F_E(\beta))} \left(e^{-2\beta(F_S(2\beta)-F_S(\beta))} \right. \\ & - 2e^{-3\beta(F_S(3\beta)-F_S(\beta))} + e^{-4\beta(F_S(2\beta)-F_S(\beta))} \Big) \\ & + e^{-2\beta(F_S(2\beta)-F_S(\beta))} [C_S(2\beta)/(4k_B\beta^2) \\ & + (U_S(2\beta) - U_S(\beta))^2] (\Delta b)^2, \end{aligned} \quad (10)$$

where $\Delta b = b - \beta$, k_B is the Boltzmann factor, $C_S(n\beta)$ and $U_S(n\beta)$ are, respectively, the specific heat and average energy of the system S at inverse temperature $n\beta$. It is obvious that for the uncoupled system $b = \beta$. For the coupled system, b is not necessarily equal to β .

In order to test the perturbation theory predictions, we numerically simulate a spin-1/2 system divided into a system S and an environment E in a canonical state. We consider a quantum spin-1/2 model defined by the Hamiltonian of Eq. (1) where

$$H_S = - \sum_{i=1}^{N_S-1} \sum_{j=i+1}^{N_S} \sum_{\alpha=x,y,z} J_{i,j}^\alpha S_i^\alpha S_j^\alpha, \quad (11)$$

$$H_E = - \sum_{i=1}^{N_E-1} \sum_{j=i+1}^{N_E} \sum_{\alpha=x,y,z} \Omega_{i,j}^\alpha I_i^\alpha I_j^\alpha, \quad (12)$$

$$H_{SE} = - \sum_{i=1}^{N_S} \sum_{j=1}^{N_E} \sum_{\alpha=x,y,z} \Delta_{i,j}^\alpha S_i^\alpha I_j^\alpha. \quad (13)$$

Here, S_i^α and I_i^α denote the spin-1/2 operators of the spins at site i of the system S and the environment E , respectively. The number of spins in S and E are denoted by N_S and N_E , respectively. The total number of spins in the whole system is $N = N_S + N_E$. The parameters $J_{i,j}^\alpha$ and $\Omega_{i,j}^\alpha$ denote the spin-spin interactions of the system S and environment E , respectively and $\Delta_{i,j}^\alpha$ denotes the local coupling interactions between spins of S and spins of E .

From Eqs. (11-13) it is clear that the Hamiltonian of the whole system, Eq. (1), obeys the symmetry properties which are required to make the first-order term of the perturbation expansion of the expectation value of σ^2 (see Eq. (7)) exactly zero. Namely, by only reversing the spin components of the system or environment spins, H_S and H_E do not change but the sign of H_{SE} reverses. Note that such a symmetry is also obeyed in the case that there is no interaction between the environment spins, *e.g.* for an environment Hamiltonian $H_E = -\sum_{i=1}^{N_E} \sum_{\alpha=x,y,z} \Omega_i^\alpha I_i^\alpha$ [26, 27]. In this particular case, it is only required that H_S is an even function and H_{SE} an odd function under reversal of all spin components of the system spins.

In our simulations we use the spin-up – spin-down basis and use units such that $\hbar = 1$ and $k_B = 1$ (hence, all quantities are dimensionless). Numerically, the propagation by $\exp(-\beta H)$ is carried out by means of exact diagonalization and the Chebyshev polynomial algorithm [28–32] with initial state $|\Psi(0)\rangle$ (see Eq. (4)). These algorithms yield results that are very accurate (close to machine precision).

Figure 1 shows the simulation results for $\langle\langle\sigma^2\rangle\rangle^{1/2}$ and $\langle\langle\delta^2\rangle\rangle^{1/2}$ obtained by exact diagonalization for the whole system $S + E$ being a spin chain with $N_S = 4$ and $N_E = 8$. The system S and environment E consist of two ferromagnetic spin chains with isotropic spin-spin interaction strengths $J_{i,j}^\alpha = J = \Omega_{i,j}^\alpha = \Omega = 1$. They are connected by one of their end-spins, with an interaction strength $\Delta_{N_S,1}^\alpha = \Delta$. The global system-environment coupling strength $\lambda = 1$. The simulation results are averaged over 1000 runs with different initial random states. Substituting the numerically obtained values for the free energy of the system and environment for $\lambda\Delta = 0$ in the analytical expressions for $\langle\langle\sigma^2\rangle\rangle^{1/2}$ and $\langle\langle\delta^2\rangle\rangle^{1/2}$ given by Eq. (8) and Eq. (10), respectively, results in the solid lines depicted in Fig. 1. It is clear that the simulation results for the uncoupled system ($\lambda\Delta = 0$) and for the coupled cases when $(\beta J)^{-1} \gtrsim 6\lambda\Delta$ agree with the analytical results for the whole range of temperatures. As the temperature decreases, the state of the whole system $S + E$ approaches the ground state, $\langle\langle\sigma^2\rangle\rangle$ becomes constant, its numerical value being given by Eq. (9). For the case at hand, $g_S = 5$, $g_E = 9$, $D_S = 16$ and $D_E = 256$ and Eq. (9) yields $\langle\langle\sigma^2\rangle\rangle^{1/2} = 0.21$, in excellent

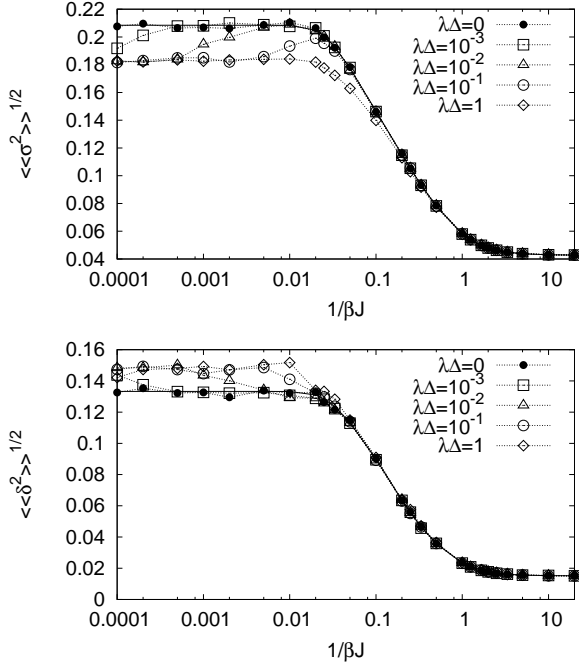


FIG. 1. Simulation results for $\langle\langle\sigma^2\rangle\rangle^{1/2}$ and $\langle\langle\delta^2\rangle\rangle^{1/2}$ for spin-1/2 chains with $N_S = 4$, $N_E = 8$, $J = \Omega = 1$ and various interaction strengths Δ as a function of the temperature $1/\beta J$. The solid lines are obtained from Eq. (8) and Eq. (10) by using numerical values for the free energies $F_S(n\beta)$ and $F_E(n\beta)$. The dotted lines are guides to the eye.

agreement with the numerical data. In the coupled case and for small $1/\beta J$, $\langle\langle\sigma^2\rangle\rangle^{1/2}$ develops a plateau different from that of the uncoupled case. The dependence of this plateau on β or $\lambda\Delta$ is nontrivial, requiring a detailed analysis of how the ground state of $S + E$ leads to the reduced density matrix of S (in the basis that diagonalizes H_S). In this respect, the β or $\lambda\Delta$ dependence of the data show in Fig. 1 are somewhat special because the ferromagnetic ground state of the system does not depend on $\lambda\Delta$.

For the spin system under study with $\lambda\Delta \neq 0$, the first-order term of the perturbation expansion of the expectation value of σ^2 in terms of $\beta\lambda\Delta$ is exactly zero. Hence, for a weakly coupled system ($\lambda\Delta$ small) deviations from the analytical results Eq. (8) and Eq. (10) obtained for the uncoupled system ($\lambda\Delta = 0$), are, as expected, seen *only* in the low temperature region. The numerical results (symbols) in Fig. 1 are in excellent agreement with the predicted results (solid lines) as long as $\beta\lambda\Delta$ is small. For a finite $\beta\lambda\Delta$, the plateaus at low temperature may or may not be reached and therefore the perturbation results are no longer applicable.

In order to study the behavior of σ and δ as a function of the global coupling interaction strength λ , we performed large-scale simulations for a spin system configured as a ring with $N_S = 4$ and $N_E = 26, 36$ at the inverse temperature $\beta|J| = 6$. This required working with a Hilbert space of size up to $D \approx 1.1 \times 10^{12}$. We assumed that the spin-spin inter-

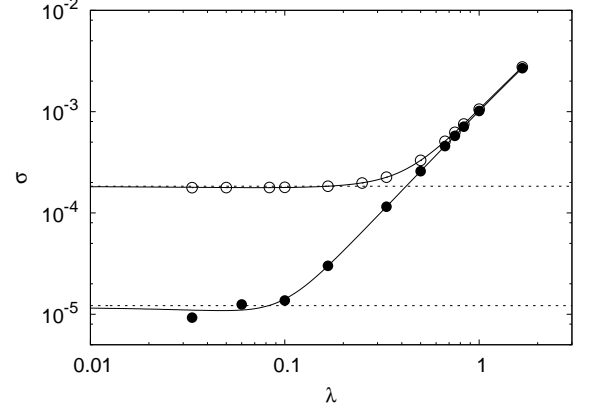


FIG. 2. Simulation results for σ for a ring with $N_S = 4$, $N_E = 26$ (open circles) and $N_S = 4$, $N_E = 36$ (solid circles) as a function of the global interaction strength λ for $\beta|J| = 6$. For the values of the interaction parameters, see text. The solid lines are fits to the data as described in the text. The top (bottom) dashed line represents the value obtained by simulating the non-interaction system ($\lambda = 0$) with 30 (40) spins.

action strengths of the system S are isotropic, $J_{i,j}^\alpha = J = -1$, that those of the environment E are only nonzero for nearest neighbors and that only $\Delta_{N_S,1}^\alpha$ and Δ_{1,N_E}^α are nonzero. The nonzero values of $\Omega_{i,j}^\alpha$ and $\Delta_{i,j}^\alpha$ are generated uniformly at random from the range $[-4/3, 4/3]$.

In Fig. 2 we present the simulation results for σ as a function of λ . Least square fitting of the data for σ^2 to polynomials in λ , we find that a polynomial of degree 7th yields the best fit, for both the 30- and 40-spin system data [33, 34]. The behavior of δ is very similar to that of σ and is therefore not shown. From Fig. 2 it is clear that for $\lambda \approx 1$, the scaling of σ with the dimension of the Hilbert space of the environment is almost completely suppressed. This is a finite temperature effect: for $\beta = 0$, this scaling property holds independent of the coupling λ [20].

Summarizing, in this Letter, we investigate the measures of decoherence and thermalization of a quantum system S coupled to an environment E at finite temperature. If the whole system $S + E$ is prepared in a canonical thermal state, we show by means of perturbation theory that σ^2 , the degree of the decoherence of S , is of the order $\beta^2 \lambda^2$. Up to the first order in the system-environment interaction we find $\sigma^2, \delta^2 \propto \exp\{-2\beta[F_E(2\beta) - F_E(\beta)]\}$ where F_E is the free energy of the environment. This provides a measure for how well a weakly-coupled specific finite environment can decohere and thermalize a system at an inverse temperature β . A measure for how difficult it is to decohere a quantum system is given by ratios of free energies of the system, and at low temperatures by $\sigma^2 \sim 1/2g_E$ for a highly degenerate ground state for S and a ground state degeneracy g_E for E . We performed numerical simulations of spin-1/2 systems to assess the region of validity of the analytical results.

Strictly speaking, the system S completely decoheres if

there is no interaction between S and E and if $N_E \rightarrow \infty$. If S is coupled to E , the S – E interaction is important. Generally, σ and δ for a finite system S are finite even in the thermodynamic limit ($N_E \rightarrow \infty$). However, if the canonical ensemble is a good approximation for the state of the system for some inverse temperatures β up to some chosen maximum energy $E_{hold} > 0$ (measured from the ground state), then it is required that $\exp(-\beta E_{hold}) \gg \sigma$. By determining the crossover of the left- and right-side functions, we find a threshold for the temperature above which the state of the system is well approximated by a canonical ensemble, and below which quantum coherence of the system is well preserved.

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 - [34] The coefficients of the 7th-order polynomial fit to the data (see Fig. 2) of the 40-spin system are $a_0 = 0.14 \times 10^{-9}$, $a_1 = -0.65 \times 10^{-9}$, $a_2 = 0.27 \times 10^{-8}$, $a_3 = -0.12 \times 10^{-7}$, $a_4 = 0.11 \times 10^{-5}$, $a_5 = 0.46 \times 10^{-8}$, $a_6 = -0.80 \times 10^{-7}$, and $a_7 = 0.12 \times 10^{-7}$.